



# **Advances in Self-Consistent Accelerator modeling: status report**

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Presented at FNAL

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# Advances in Self-Consistent Electromagnetic Modeling

- Complex cavity computations with particles have been improved through algorithms, including parallelization, making possible computations of wakefields in complex structures, intrabunch effects, injectors, ...
- Summary of some of what has made this possible
  - Local charge and current deposition methods
  - Parallelization
  - Improved stability
  - Boundary representations
- Comparison with
  - Finite element approaches
  - Unitary separation approaches

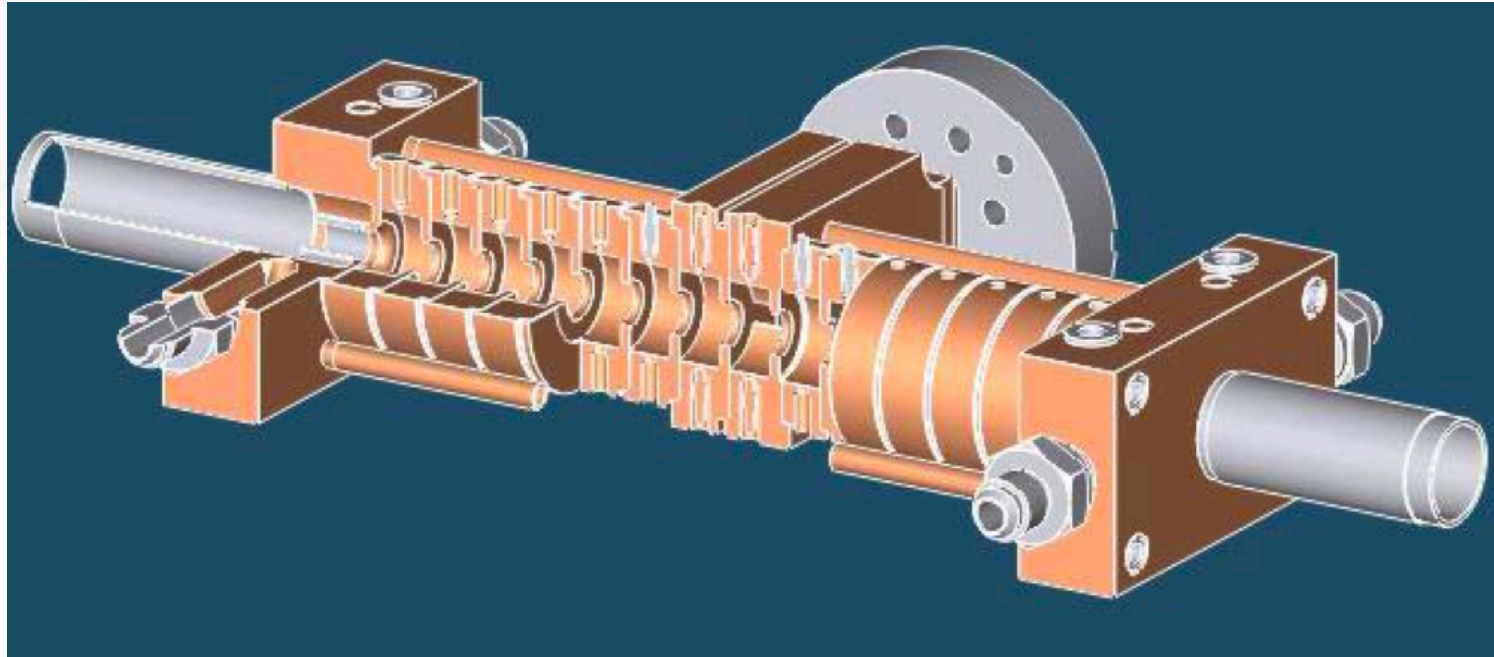


# The goals of modeling?

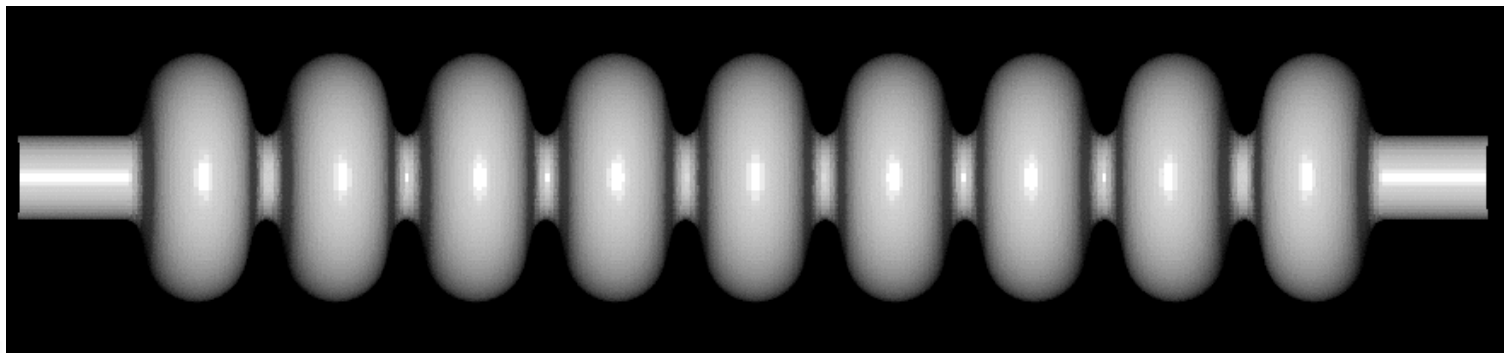
- Part of the design process
  - Create
  - Simulate
  - Build
  - Test
- Simulation for prediction of
  - Cavity losses
  - Instability
- In general for
  - Exploration
  - Confirmation
  - Elucidation



**Modeling allows one to answer questions  
without construction cost**



**NLC**



**ILC (Tesla)**



# Basic problem in charge particles moving in EM fields

- Maxwell

$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E}$$

$$\frac{\partial \mathbf{E}}{\partial t} = c^2 [\nabla \times \mathbf{B} - \mu_0 \mathbf{j}]$$

- Particle sources

$$\mathbf{j} = \sum q_i \mathbf{v}_i \delta(\mathbf{x} - \mathbf{x}_i)$$

- Particle dynamics

$$\frac{d(\gamma \mathbf{v})}{dt} = \frac{q_i}{m_i} [\mathbf{E}(\mathbf{x}_i, t) + \mathbf{v}_i \times \mathbf{B}(\mathbf{x}_i, t)]$$

$$\frac{d\mathbf{x}_i}{dt} = \mathbf{v}_i$$

Auxiliary equations

$$\nabla \cdot \mathbf{B} = 0$$

$$\nabla \cdot \mathbf{E} = \rho / \epsilon_0$$

$$\rho = \sum q_i \delta(\mathbf{x} - \mathbf{x}_i)$$



## **With much other physics added for a complete model**

- Particle injection
- Dark currents
- Multipactoring
- Photon (short wavelength) production
- Surface resistance
- Secondary emission



# **ELECTROMAGNETICS**





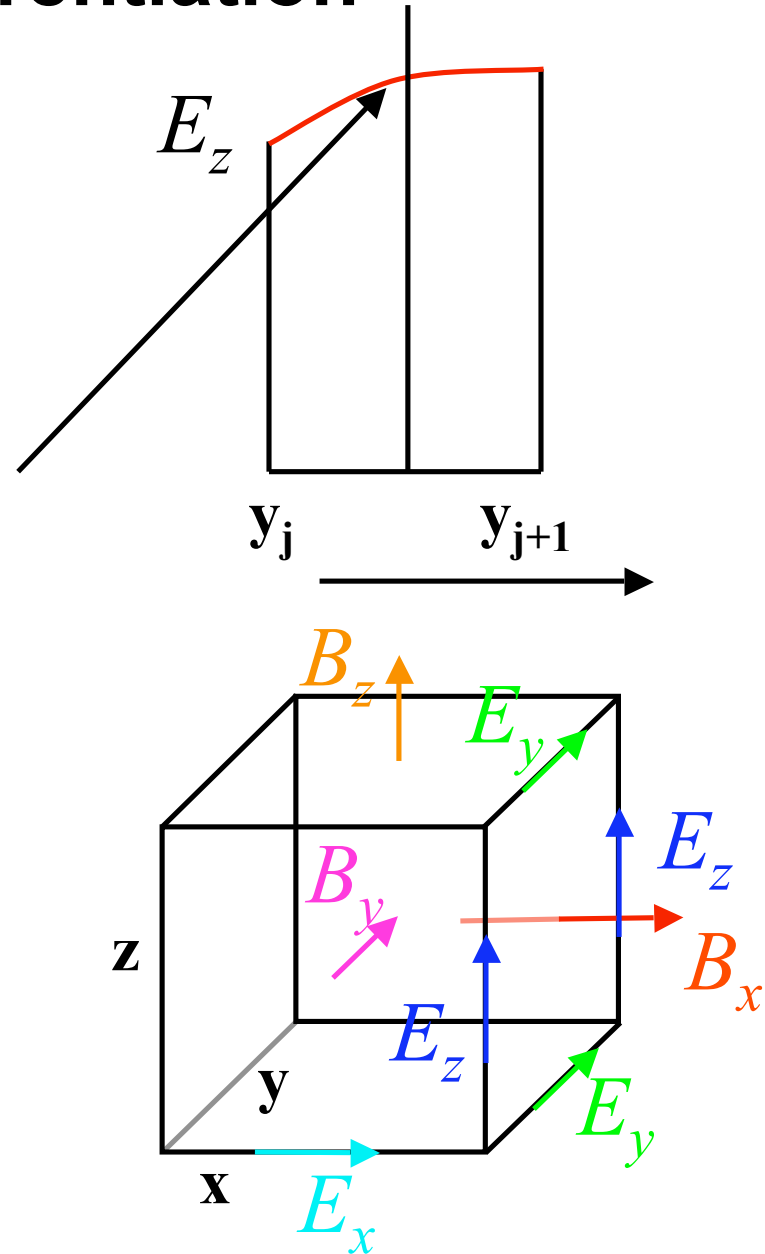
## Yee: 2nd order accurate spatial differentiation

$$\frac{\partial B_x}{\partial t} = -\frac{\partial E_z}{\partial y} + \frac{\partial E_y}{\partial z}$$

- At the midpoint

$$\frac{\partial E_z}{\partial y} = \frac{E_{z,j+1} - E_{z,j}}{\Delta y} + O(\Delta y^2)$$

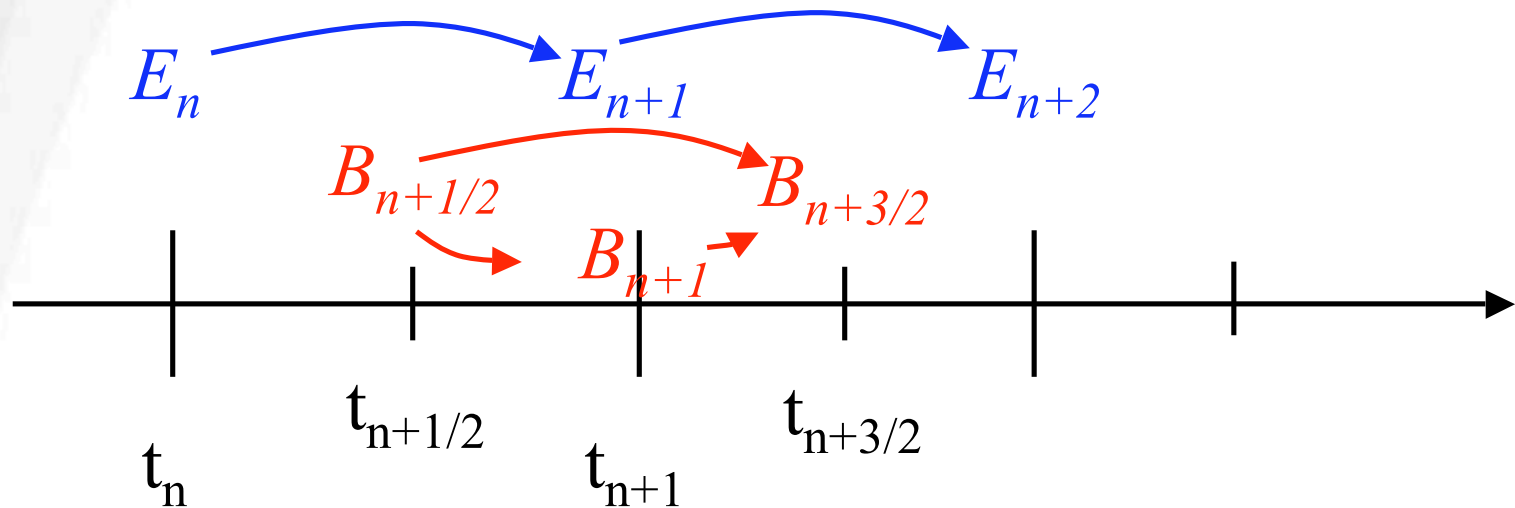
- Leads to special layout of values in a cell
- *Yee mesh* gives 2nd order accuracy of spatial derivatives







## Second-order in time by leap frog



$$\frac{\partial B_x}{\partial t} = -\frac{\partial E_z}{\partial y} + \frac{\partial E_y}{\partial z}$$

$$B_{x,i,j,k}^{n+1/2} - B_{x,i,j,k}^{n-1/2} = \Delta t \left( \frac{E_{z,i,j,k}^n - E_{z,i,j+1,k}^n}{\Delta y} + \frac{E_{y,i,j,k+1}^n - E_{y,i,j,k}^n}{\Delta z} \right)$$

- Time centered differences give second order accuracy in  $\Delta t$
- Can get time-collocated values by half-stepping in B
- Similar for E update, except  $c^2$  factor



## Matrix representation useful for stability

$$\frac{dB_{x,i,j,k}}{dt} = \left( \frac{E_{z,i,j,k} - E_{z,i,j+1,k}}{\Delta y} + \frac{E_{y,i,j,k+1} - E_{y,i,j,k}}{\Delta z} \right)$$

$$\frac{d\mathbf{b}}{dt} = -\mathbf{C} \cdot \mathbf{e} \quad \frac{d\mathbf{e}}{dt} = c^2 \mathbf{C}' \cdot \mathbf{b} \quad \frac{d^2 \mathbf{b}}{dt^2} = -c^2 \mathbf{C} \cdot \mathbf{C}' \cdot \mathbf{b} = -\mathbf{D} \cdot \mathbf{b}$$

- Magnetic and electric spaces are different
- $\mathbf{C}$ ,  $\mathbf{C}'$  are adjoints, so  $\mathbf{D}$  is self-adjoint (symmetric)
- Diagonalize into separate harmonic oscillators
- Leap frog for harmonic oscillator, stability limit at

$$\omega_{\max} \Delta t_{CFL} = 2 \quad \Delta t_{CFL} = \frac{1}{c \sqrt{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}}}$$



## Gershgorin Circle Theorem gives stability bound

- Frequencies are eigenmodes of  $D = c^2 C' C$
- Eigenvalues in range

$$0 < \omega^2 < \max \left( \sum_j |D_{ij}| \right) \text{ over } i$$

- Gives precise range for infinite grid
- Points to relation between coefficients and frequencies for other cases



## Many other methods available

- Finite element - later
- Hamiltonian splitting (de Raedt): into exactly solvable parts
$$\frac{d(\mathbf{b}, \mathbf{e})}{dt} = \mathbf{A} \bullet (\mathbf{b}, \mathbf{e}) = \mathbf{M} \bullet \mathbf{N} \bullet (\mathbf{b}, \mathbf{e})$$
  - known:  $\frac{d\mathbf{U}_M}{dt} = \mathbf{M} \bullet \mathbf{U}_M$     $\frac{d\mathbf{U}_N}{dt} = \mathbf{N} \bullet \mathbf{U}_N$
  - stable approximate solution (since unitary):
$$\mathbf{U}(\Delta t) = \mathbf{U}_N(\Delta t / 2) \bullet \mathbf{U}_M(\Delta t) \bullet \mathbf{U}_N(\Delta t / 2)$$
  - Similar to drift-kick of symplectic integration
- *None of these has yet proven as effective for self-consistent particle simulation as FDTD, explicit or implicit*



# PARTICLES



# Computing particle-particle interactions is prohibitive

- Coulomb interaction leads to  $N_p^2$  force computations

$$\frac{d\gamma_i \mathbf{v}_i}{dt} = \frac{q_i}{\epsilon_0 m_i} \sum_j q_j \frac{\mathbf{x}_i - \mathbf{x}_j}{|\mathbf{x}_i - \mathbf{x}_j|^3}$$

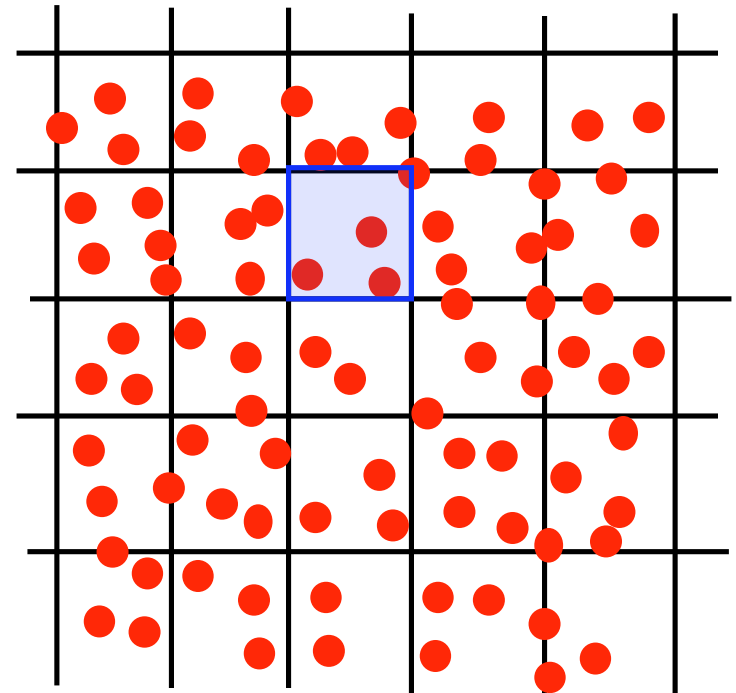
- Lenard-Weichert (retarded potentials) - worse due to need to keep history

$$\frac{d\gamma_i \mathbf{v}_i}{dt} = \frac{q_i}{\epsilon_0 m_i} \sum_j q_j \mathbf{F}_{ij}(\mathbf{x}_i, \mathbf{x}_j(t - \tau))$$



## Particle In Cell (PIC) reduces to $N_p$ scaling

- Particle contributions to charges and currents are added to each cell:  $O(N_p)$  operations
- Forces on a particle are found from interpolation of the cell values:  $O(N_p)$  operations

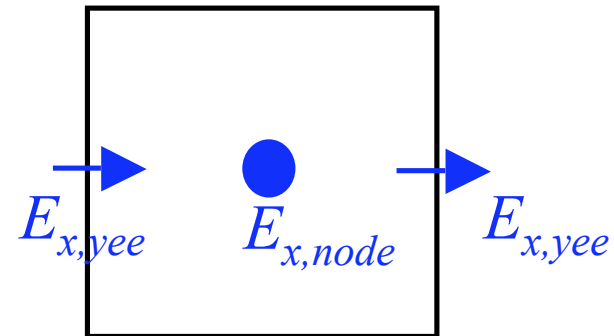
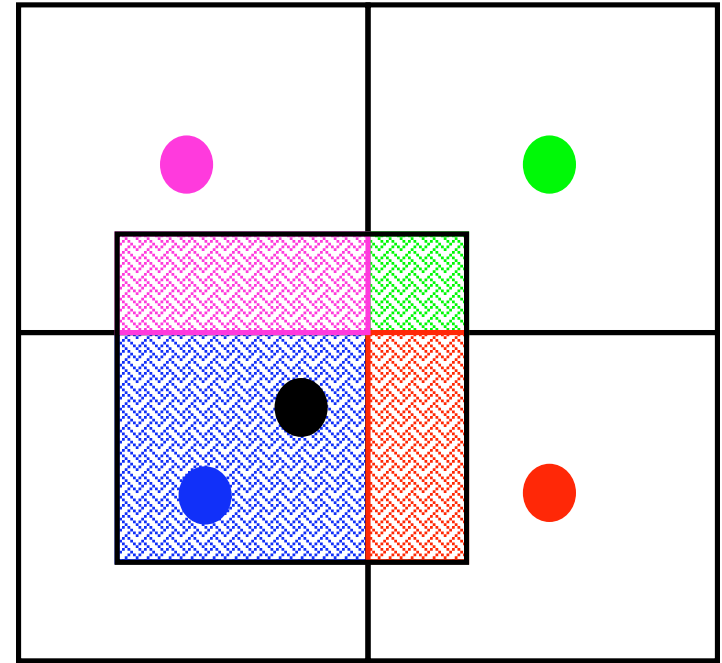






## Finding the force: interpolation (gather)

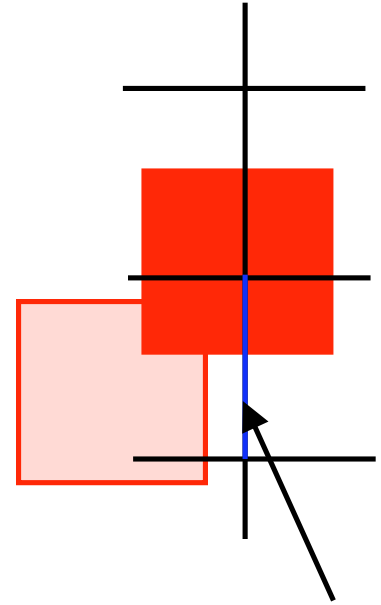
- Linear weighting for each dimension
  - 1D: linear
  - 2D: bilinear = area weighting
  - 3D: trilinear = volume weighting
- Force obtained through 1st order, error is 2nd order
- For simplicity, no loss of accuracy, weight first to nodal points



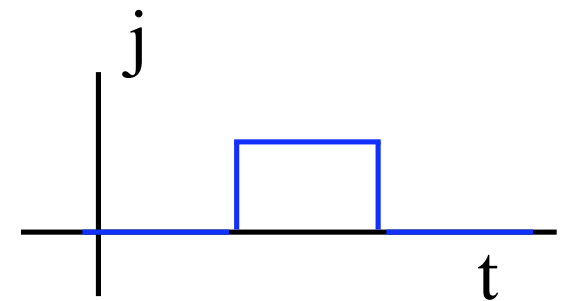


# A special scatter ensures finite difference charge conservation

- Principle: apportion via some weighting
- Computing the charge density
  - Compute the current density and find the charge density from finite difference
  - Directly weight particles to the grid
- If these two methods do not agree, then one can have false charge buildup from the Ampere-Maxwell equation. Requires Poisson solve to remove.
- Villasenor/Buneman explicitly conserves charge, but is noisier



Current contrib. to this interface must match charge difference change across separated cells



# Mardahl and Verboncoeur show importance of getting this right

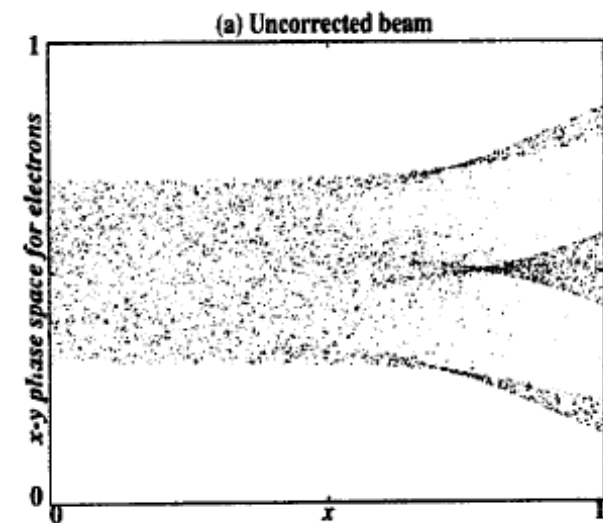
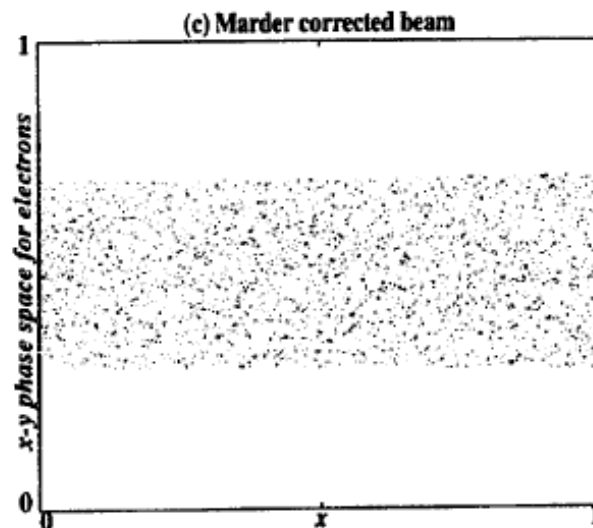
ELSEVIER

Computer Physics Communications 106 (1997) 219–229

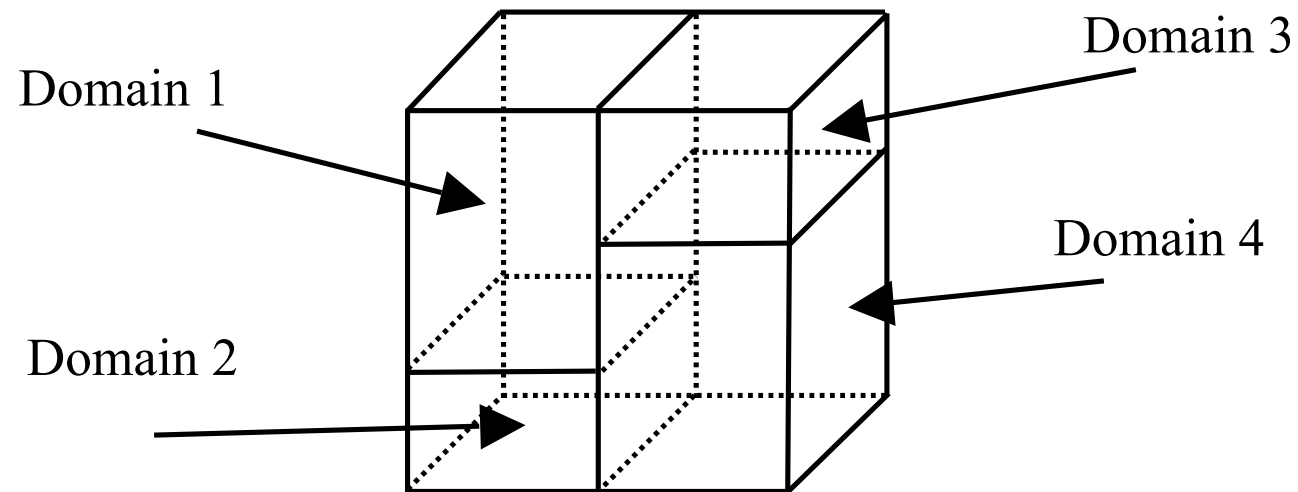
## Charge conservation in electromagnetic PIC codes; spectral comparison of Boris/DADI and Langdon–Marder methods

P.J. Mardahl<sup>1</sup>, J.P. Verboncoeur*Cory Hall Box 173, Department of Electrical Engineering and Computer Science, University of California, Berkeley, CA 94720-1770, USA*

Received 1 April 1997; revised 11 August 1997



## Parallelism: domain decomposition





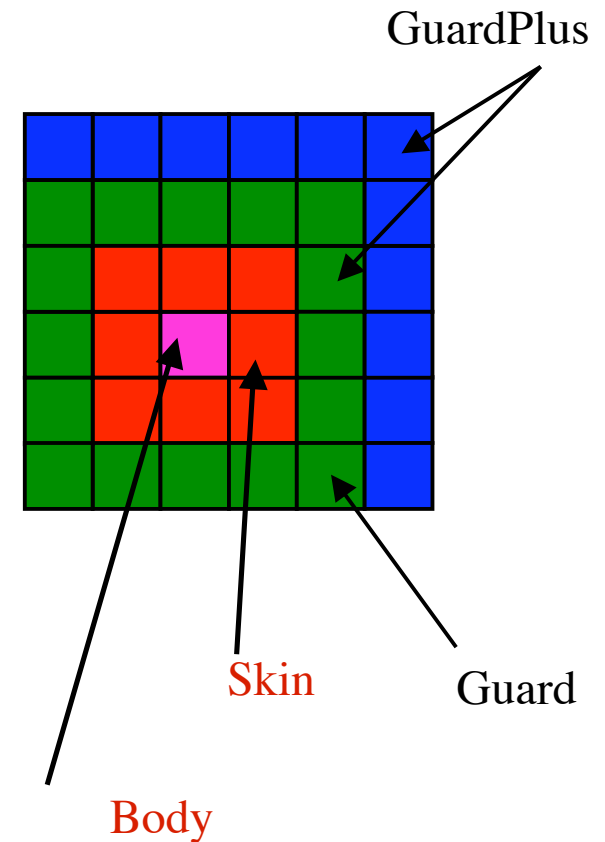
## Parallelism rules of thumb

- Communication is expensive
- Global solves are really expensive



# Overlap of communication and computation needed for speed

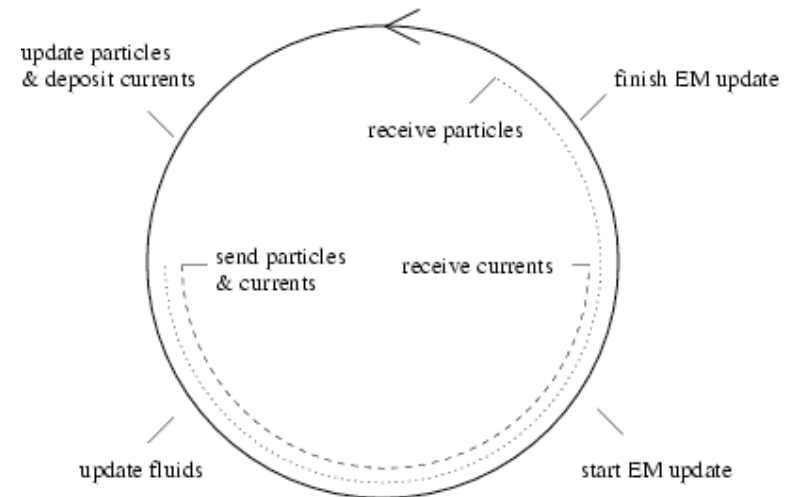
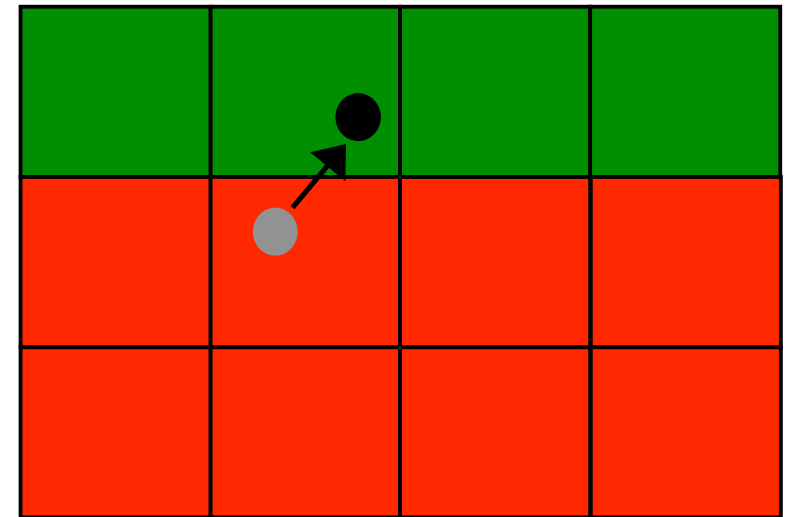
- Non overlap algorithms:
  - Compute domain
  - Send skin (outer edge)
  - Receive guard
  - Repeat
- Overlap algorithms
  - Compute skin
  - Send skin
  - Compute interior
  - Receive guard
  - Repeat





## Similar overlap possible for particles

- Move particles and weight currents to grid
- Send currents needed by neighboring processors
- Send particles to neighboring processors
- Update B for half step
- Receive currents and add in
- Update E, B
- Receive particles



Without charge conserving current deposition, further costly global solve



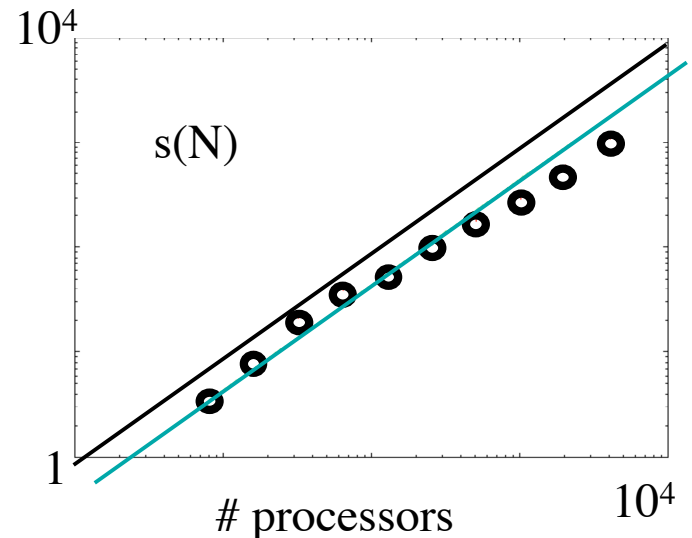


# VORPAL implements basic algorithms in highly scalable manner

## Object-oriented and flexible

(Arbitrary dimensional)

- Self-consistent EM modeling
  - Full EM or electrostatic + cavity mode
  - Particle in cell with relativistic or nonrelativistic dynamics
- But has other capabilities
  - Impact and field ionization
  - Fluid methods for plasma or neutral gases
  - Implicit EM
  - Secondary emission
- And is modern
  - Serial or Parallel (general domain decomposition)
  - Cross-platform (Linux, AIX, OS X, Windows)
  - Cross-platform binary data (HDF5)



**VORPAL scales well to  
1,000's of processors  
(strong scaling)**



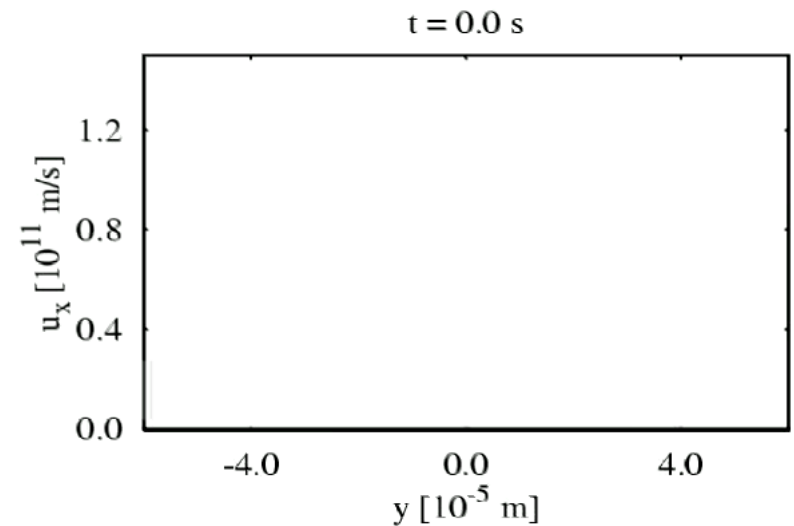
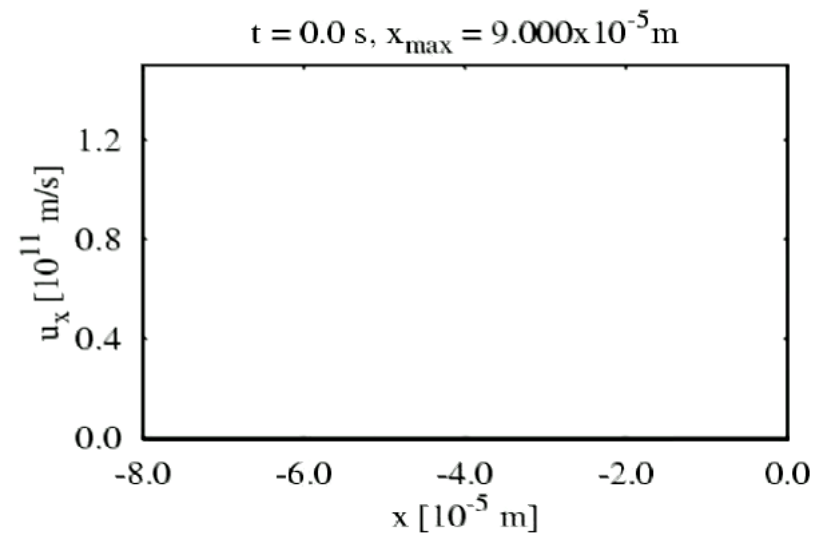
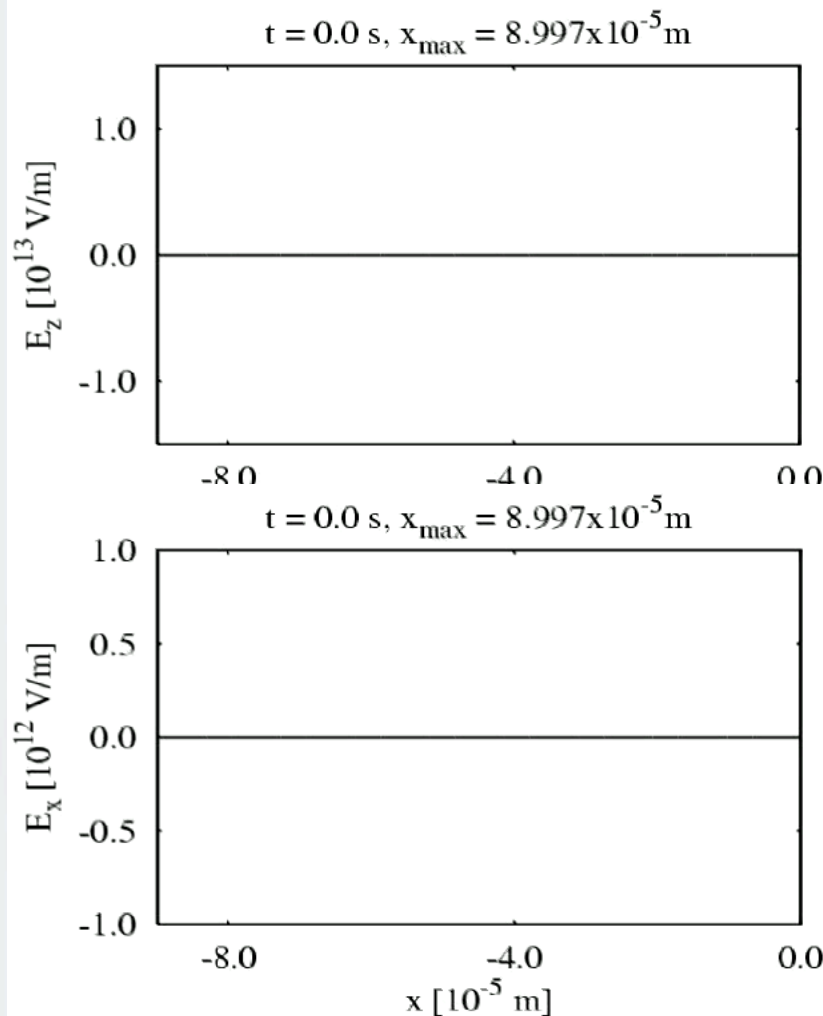
# Simplest algorithm allows complex computations

- Example: formation of beams in laser-plasma interaction





# Elucidation: long pulses shorten to resonance, capture, loading, acceleration



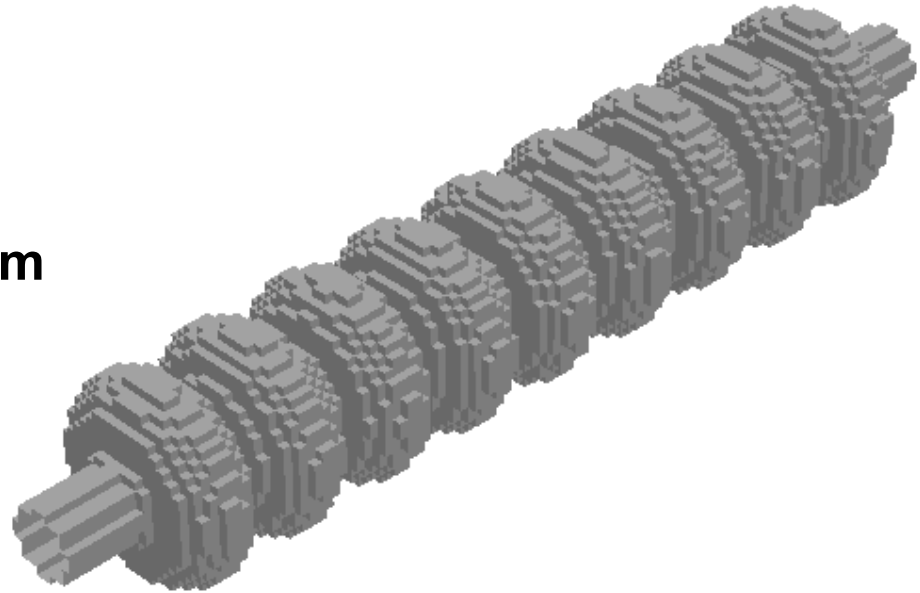


## **Complications: boundaries**



## Early work on structured meshes had *stair-step* boundary conditions

**$120 \times 24 \times 24 = 71,424$  cells  
= 215,000 degrees of freedom**

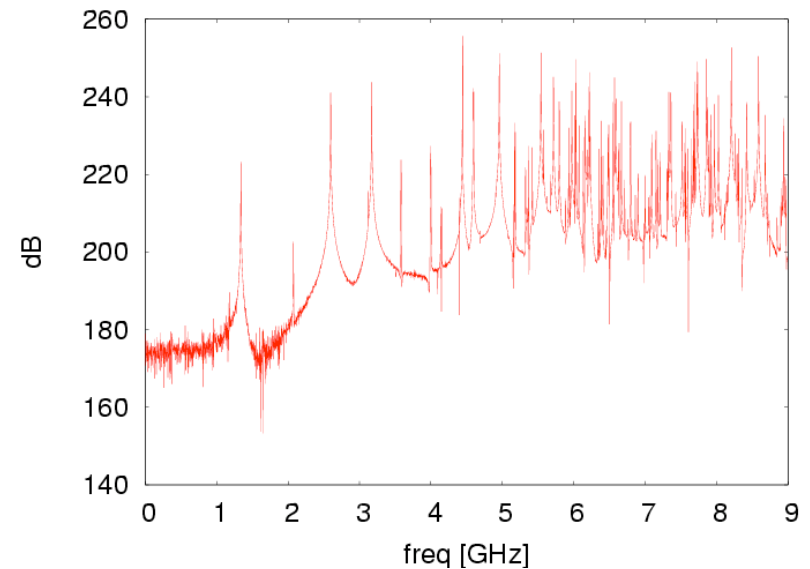


- $N (L/\Delta x)$  cells in each direction
- Error of  $(\Delta x/L)^3$  at each surface cell
- $O(N^2)$  cells on surface
- Error =  $N^2(\Delta x/L)^3 = O(1/N)$



# Modes computed with combination of FFT and fitting

- 3 cell SRF
- High density of higher-order modes
- FFT allows extraction of field shape
- Excite that field, measure frequency by fitting

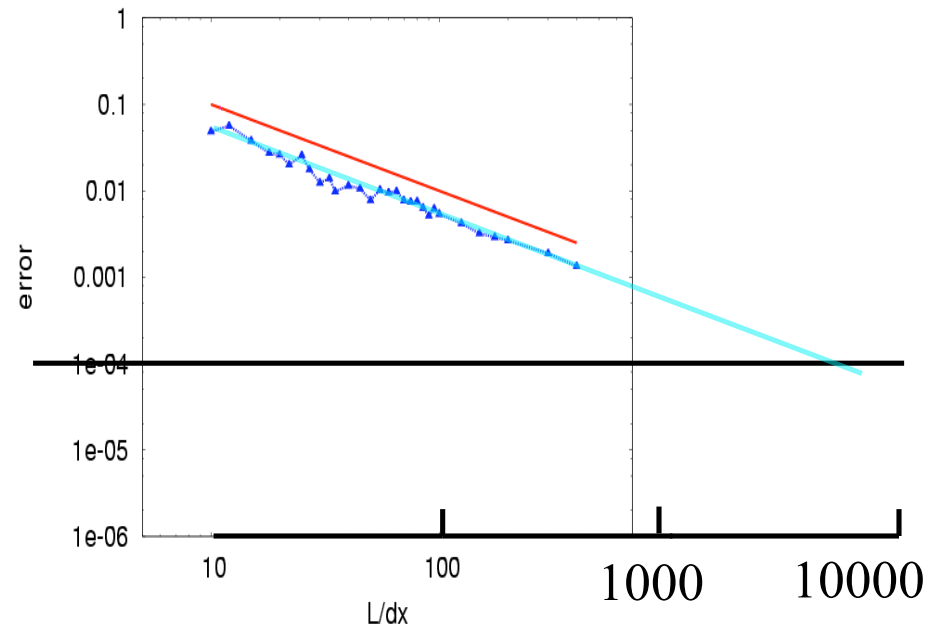


**Excite with delta-function initial condition  
Run 25000 steps  
FFT**



## Convergence studies confirm result, indicate modeling problem

- Stair-step error is  $10^{-3}$  at 1000 cells per dimension, error linear with cell size
- Requires 10,000 cells per dimension to get  $10^{-4}$  accuracy
- $10^{12}$  cells for 3D problem



This approach will not give answer even on large, parallel hardware





## Finite elements give one approach to improved boundary modeling

- Tau3P, HFSS, ...

$$\mathbf{B} = \sum b_k(t) \mathbf{u}_k^B(x) \quad \mathbf{E} = \sum e_\ell(t) \mathbf{u}_\ell^E(x)$$

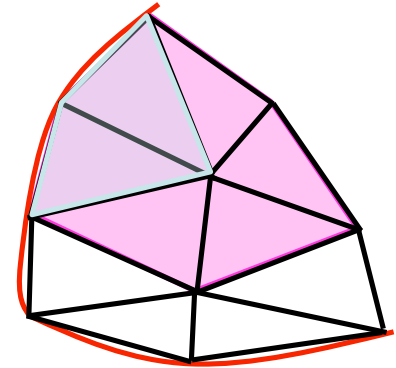
$$\frac{\partial \mathbf{B}}{\partial t} = \sum \frac{db_k}{dt}(t) \mathbf{u}_k^B(x) \quad \nabla \times \mathbf{E} = \sum e_\ell(t) \nabla \times \mathbf{u}_\ell^E(x)$$

$$\sum \frac{db_k}{dt}(t) \mathbf{u}_k^B(x) = - \sum e_\ell(t) \nabla \times \mathbf{u}_\ell^E(x)$$

$$\int d^3x \sum_k \frac{db_k}{dt}(t) \mathbf{u}_{k'}^B(\mathbf{x}) \mathbf{u}_k^B(\mathbf{x}) = - \int d^3x \sum_\ell e_\ell(t) \mathbf{u}_{k'}^B(\mathbf{x}) \cdot \nabla \times \mathbf{u}_\ell^E(\mathbf{x})$$

$$\mathbf{M}_b \cdot \frac{d\mathbf{b}}{dt} = -\mathbf{C} \cdot \mathbf{e}$$

$$\mathbf{M}_e \cdot \frac{d\mathbf{e}}{dt} = c^2 \mathbf{C}' \cdot \mathbf{b}$$





## Finite elements require global solves, more intense particle calculations

- Global mass matrix inversion required at each step

$$\mathbf{M}_b \cdot \frac{d\mathbf{b}}{dt} = -\mathbf{C} \cdot \mathbf{e}$$

- Self consistency difficult and charge conservation not guaranteed

$$\mathbf{M}_e \cdot \frac{d\mathbf{e}}{dt} = c^2 (\mathbf{C}' \cdot \mathbf{b} - \mu_0 \mathbf{j})$$

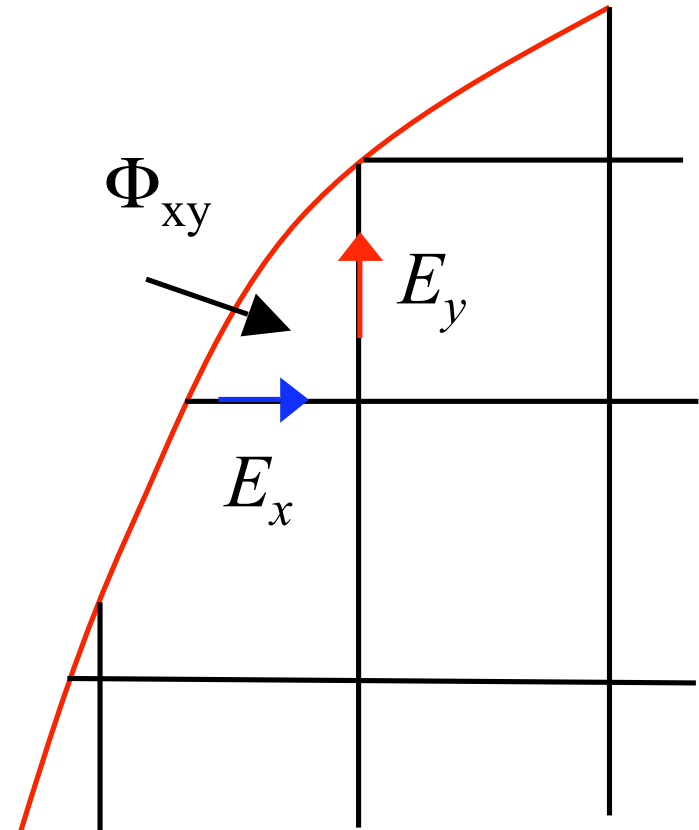
$$j_\ell = \sum_{ptcls\ i} q_i \mathbf{v}_i \mathbf{u}_\ell^E(\mathbf{x}_i((n+1/2)\Delta t))$$

- Difficult to follow particles
  - List of regions
  - List of FE's with support in that region
  - Complex FE element evaluation at each time step for each particle



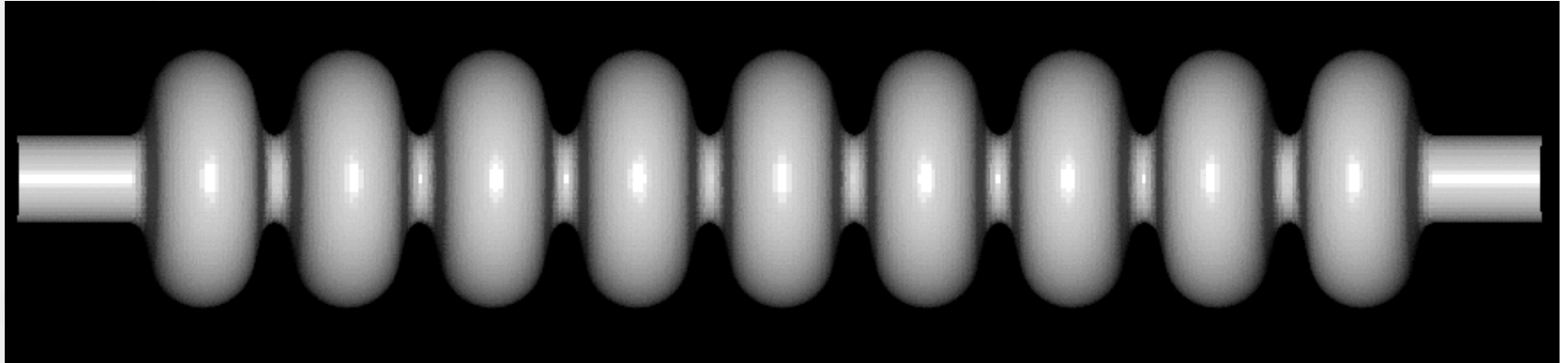
## Resurgence of regular grids: cut cells give same accuracy as finite elements

- For cells fully interior, us regular update
- For boundary cells:
  - Store areas and lengths
  - Update fluxes via
$$\dot{\Phi}_{xy} = -E_x \ell_x - E_y \ell_y$$
  - Update fields via
$$B_z = \Phi_{xy} / A_{xy}$$

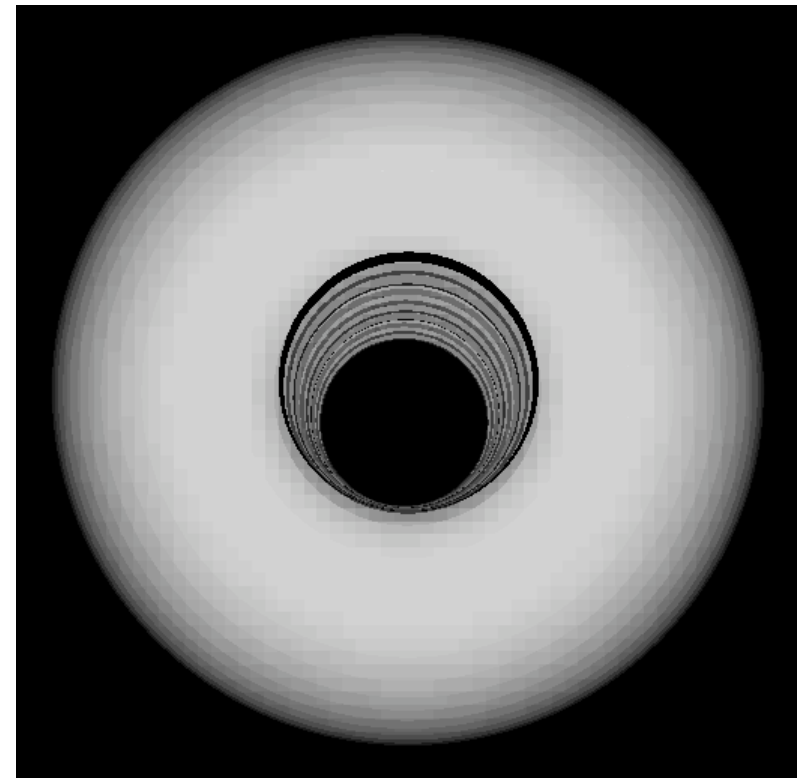




## Cut-cell boundary conditions accurately represent geometry



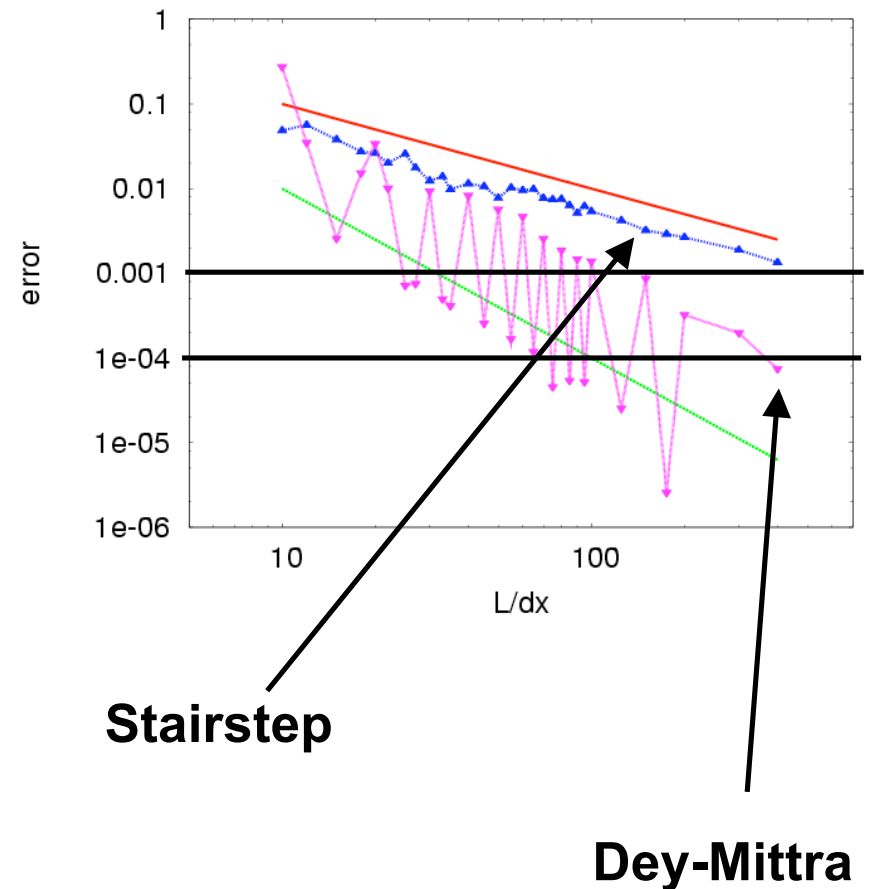
- Tesla 2000 cavities
- 312x56x56 ( $10^6$ ) cells





## Dey-Mittra (1997) cut-cells allow $10^{-4}$ accuracy

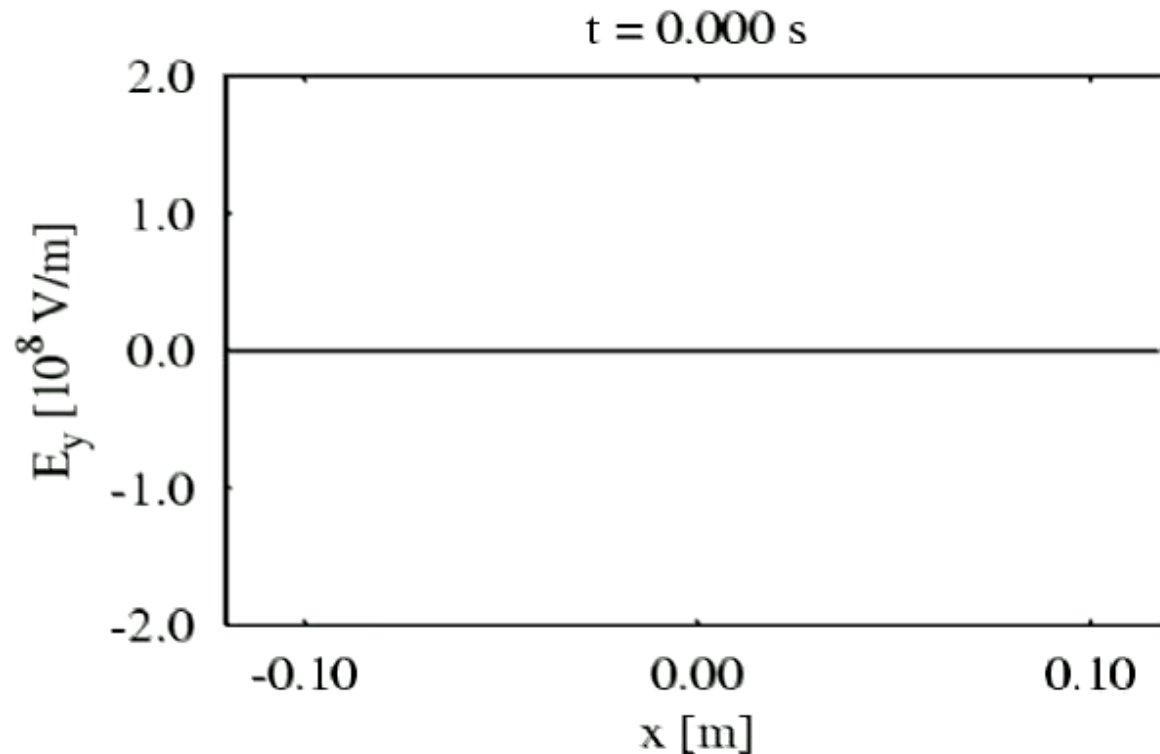
- Less than  $10^9$  cells for cavity modeling at one part in  $10^4$
- Implementation exists now in VORPAL





## Dey-Mittra problem: small triangles give high frequencies, small time steps

- B update matrix coefs  $\sim$  length/area
- Length/area becomes infinite as area vanishes
- Get localized, high-frequency modes
- Must throw out small cell fragments

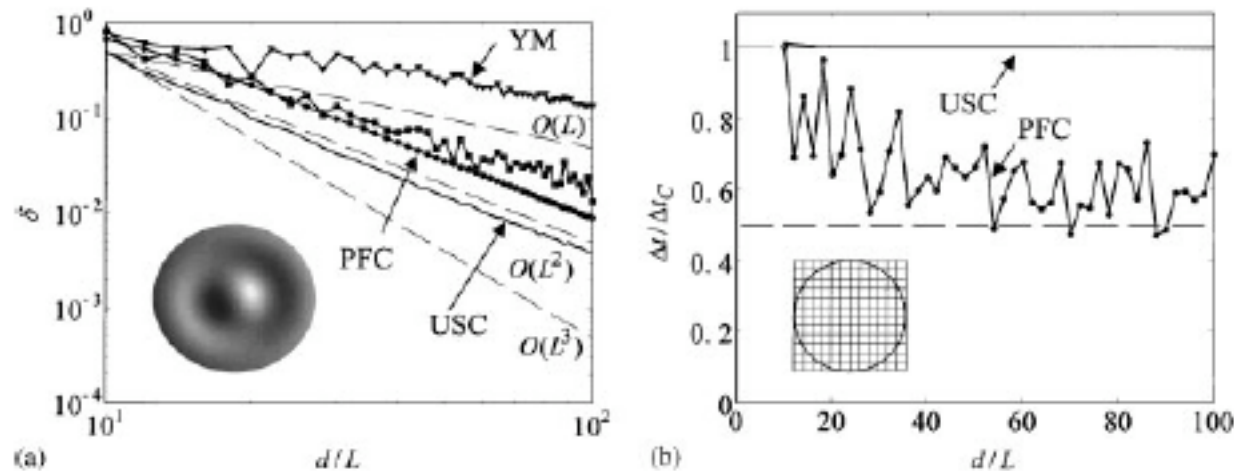


# Improvement on cut-cell recently discovered

INTERNATIONAL JOURNAL OF NUMERICAL MODELLING: ELECTRONIC NETWORKS, DEVICES AND FIELDS  
*Int. J. Numer. Model.* 2003; 16:127–141 (DOI: 10.1002/jnm.488)

## A uniformly stable conformal FDTD-method in Cartesian grids

I. A. Zagorodnov<sup>\*,†</sup>, R. Schuhmann and T. Weiland

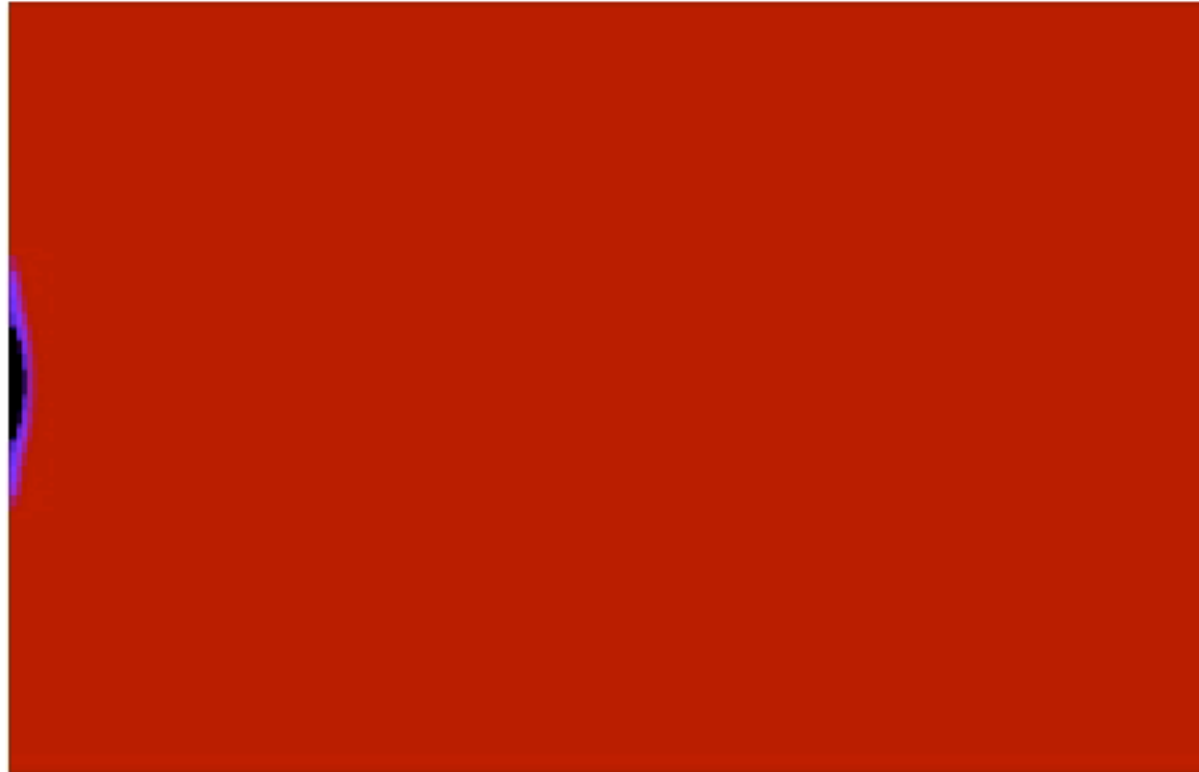


- New method gives error lower than Dey-Mittra
- Does not have reduction of stable  $\Delta t$
- Favorable properties re particle introduction
- Now being implemented





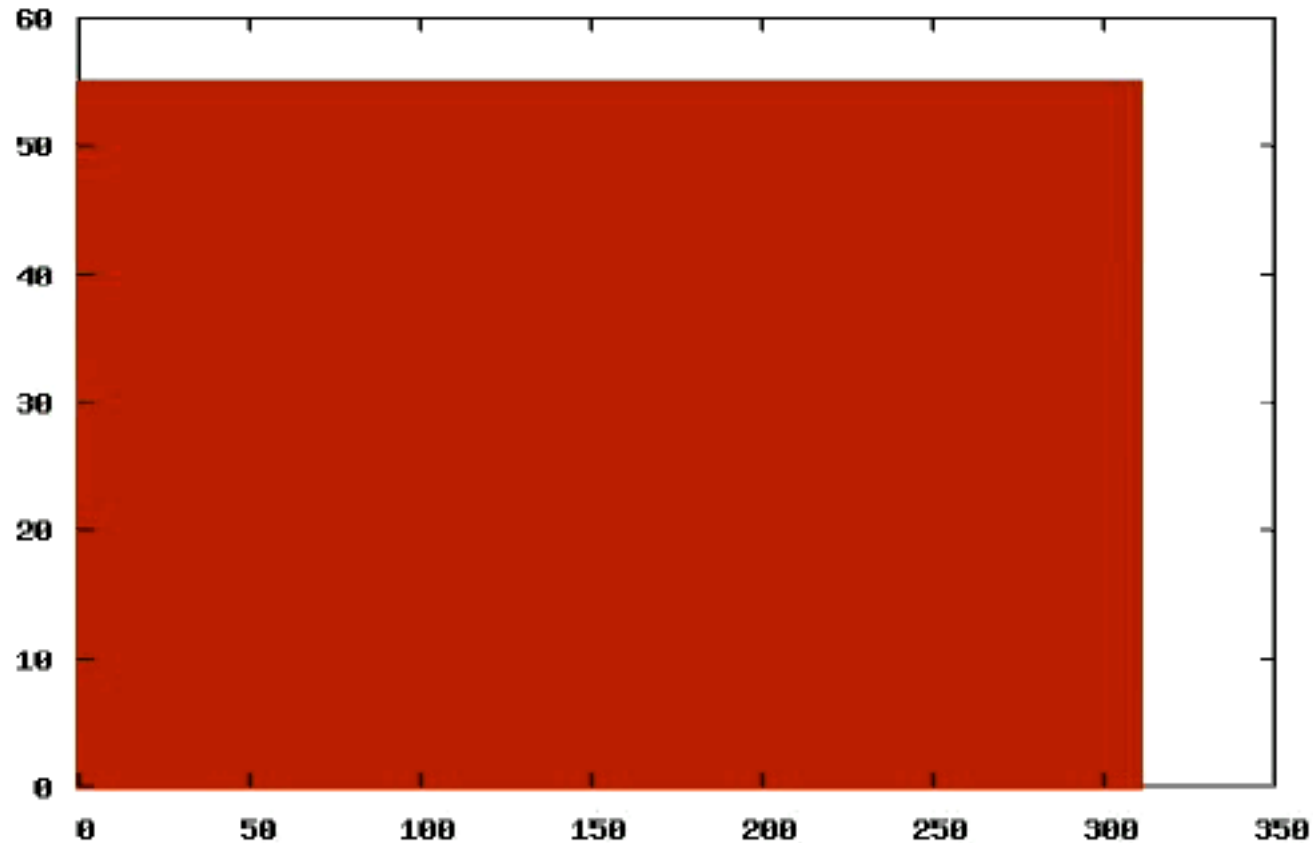
**Regular, structured grids allow for self-consistent integration of particles**



**Wakefield for NLC cavities computed by VORPAL in 3D<sub>7</sub>**



## Regular, structured grids allow for self-consistent integration of particles



Wakefield for Tesla/ILC cavities computed by VORPAL<sub>38</sub>



**This capability is at FNAL now!**

- VORPAL installed



## Future?

- More accurate EM integrators with boundaries and particles? Wish list:
  - Absolutely stable, getting slow solution correct for large time steps
  - No global solves
- More accurate particle deposition not requiring higher order in all directions
- Conformal boundaries with
  - Surface resistance
  - Dark currents